

both b , and l_0 , are complicated functions of the velocity of the moving inhomogeneous medium and the reflected pulse is Doppler-shifted.

Some numerical results have been presented in Figures (1), (2) and (3), which depict the dependence of $\phi''(\omega_0)$ and $\phi s(\omega_0)$, on the velocity of the medium v , inhomogeneity parameter a' , and carrier frequency f_0 . It is seen that higher the velocity of the medium, smaller is the delay and distortion of the reflected pulse.

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Non-applicability of Wasastjerna potential function for heavy metal halide molecules

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A large number of potential energy functions have been used by different workers for the purpose of evaluating binding energies of diatomic molecules. Rittner (1951) suggested a potential function consisting of electrostatic, Van der Waals, polarization and an exponential type of overlap. However, due to its lengthy and complicated form, attempts have been made to find out some simpler form

of potential function while retaining all the qualities of Rittner's function. In this direction, the Wasastjerna potential function,

$$\phi = -\frac{e^2}{r} + Cr^7 \exp(-\beta r) \quad \dots (1)$$

consisting of only two terms is worth mentioning. This potential function has been tried by Varshni & Shukla (1963) for predicting physical parameters of alkali hydride molecules. Likewise, Gohel (1968) has tested the applicability of this potential function to the case of alkali halide molecules. All this goes to suggest that the repulsive term $Cr^7 \exp(-\beta r)$ of the Wasastjerna function is adequate enough to represent the combined effect of polarization, Van der Waals and pure repulsion in the case of alkali hydride and alkali halide molecules. In view of this, it was thought desirable to enquire whether the Wasastjerna function could also be applied to heavy metal halides which are known to have a significant Van der Waals potential and polarization effects. For this purpose, we have calculated the binding energies of heavy metal halides by using Wasastjerna function and then compared these values with the observed values.

The potential parameters C and β appearing in eq. (1) may be evaluated from the following well-known conditions.

$$(d\phi/dr)_{r=r_e} = 0, \quad \dots (2)$$

and

$$(d^2\phi/dr^2)_{r=r_e} = K_e, \text{ the force constant} \quad \dots (3)$$

The binding energy can be calculated from the relation given by Varshni & Shukla (1965),

$$D_t = -\phi(r_e). \quad \dots (4)$$

Applying eqs. (1), (2) and (3) in eq. (4), we obtain for the binding energy,

$$D_t = \frac{e^2}{r_e} \left[1 - \frac{1}{(\beta r_e - 7)} \right] \quad \dots (5)$$

The values of the molecular constants r_e and K_e used in the calculations have been collected from various sources e.g., Kachhava & Saxena (1963) and the experimental values of binding energies have been taken from Thakur (1975). The significant difference between the calculated and experimental values of the binding energies, as evident from Table 1, indicates the inadequacy of the repulsive term in the Wasastjerna potential function to simulate the combined effect of polarization, Van der Waals and pure repulsion in its entirety in the case of heavy metal halide molecules, unlike in the case of alkali halide and alkali hydride molecules. The Wasastjerna potential function is, therefore, not

successful in the case of heavy metal halides. However, this does not simply that all two-term functions are inapplicable to heavy metal halides. The simple two-term logarithmic function,

$$\phi = -\frac{e^2}{r} + D \log(4+d/r) \quad (6)$$

as used by Pant (1976) has been found to be very successful for heavy metal halide molecules.

Table 1. Force constants (K_e), internuclear separations (r_e) and binding energies of heavy metal halide molecules.

Molecule	K_e (10^5 dyne/cm)	r_e (Å)	Calc. Binding Energy (K J mole ⁻¹)	Expt. Binding Energy (K J mole ⁻¹)
TlF	2.310	2.0844	604.90	645.6
TlCl	1.453	2.4848	521.39	590.4
TlBr	1.767	2.6181	497.80	548.9
TlI	1.037	2.8135	454.48	555.5
InCl	1.586	2.4011	530.74	629.6
InBr	1.366	2.5432	501.87	519.2
InI	1.114	2.7539	471.22	509.2
GaCl	1.952	2.2017	576.73	573.2
GaBr	1.516	2.3525	537.72	568.2
GaI	1.232	2.5747	493.50	543.9

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